

On the possibility of fusion reactions in water molecules*

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The probability of nuclear transitions $p + p + {}^{16}\text{O} \rightarrow {}^{18}\text{Ne}(4.522, 1^-)$ in molecular water is estimated. Due to the practically exact agreement of the energy of the Ne resonance and of the $p + p + {}^{16}\text{O}$ threshold, the transition probability is found to be considerably enhanced. This indicates the possibility of nuclear fusion in rotationally excited H_2O molecules of angular momentum 1^- .

Nuclear states with binding or resonance energies close to breakup thresholds have a large spatial extension due to the long tail of the corresponding wave functions. For instance, the ground state of the nucleus ${}^8\text{B}$, i.e., of the main source of high-energy solar neutrinos [1], is separated from the $p + {}^7\text{Be}$ threshold by only 130 keV. Integrations up to 300 fm, hence, are needed [2] when treating the process $p + {}^7\text{Be} \rightarrow {}^8\text{B} + \gamma$.

In nuclear reactions, the existence of near-threshold intermediate states leads to a considerable increase of the transition probability. As an example we recall the muon-catalyzed dt fusion in the molecule $(dt\mu)$, which takes place primarily via the mechanism

$$d + t \rightarrow {}^5\text{He}(3/2^+) \rightarrow {}^4\text{He} + n.$$

Since the difference between the energies of the dt threshold and the ${}^5\text{He}(3/2^+)$ resonance is only about 50 keV, it is not surprising that the probability of this process exceeds at least by four orders of magnitude the probability of nuclear transitions in the $(dd\mu)$ or $(pd\mu)$ molecules where no such resonances occur [3].

In this note we want to point to an analogous situation, however in an ordinary (electronic) molecule. From the level scheme of the nucleus ${}^{18}\text{Ne}$ [4,5] presented in Fig. 1, we infer that the measured energy $E = 4.522\text{ MeV}$ of ${}^{18}\text{Ne}(1^-)$ coincides up to the last figure with the threshold energy of the three-body channel $p + p + {}^{16}\text{O}$. Since the binding energy of the water molecule is only a few eV, this means that the rotational 1^- state of H_2O and the ${}^{18}\text{Ne}(1^-)$ state are degenerate in energy. Excited molecular water of this angular momentum, thus, is to be considered as a superposition of these pure molecular and nuclear states. In other words, the wave function of real water molecules in the 1^- state contains always an admixture of the ${}^{18}\text{Ne}(1^-)$ nuclear wave function.

The mixing coefficient of this superposition, and thus the nuclear transition probability in the H_2O molecule, is given by the overlap integral between the “pure” states. Due to

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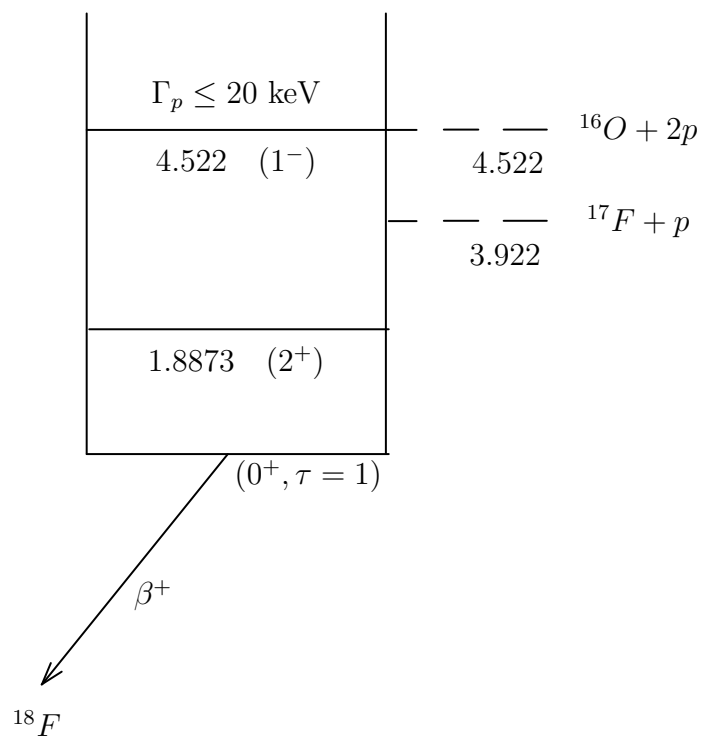


FIG. 1. Fragment of the nucleus ^{18}Ne spectrum.

the proximity of the resonance and threshold energies, intermediate and large distances (in nuclear scale) contribute considerably to this integral. As a consequence, the nuclear transition probability is enhanced, instead of being suppressed by the usual Coulomb barrier factor [6].

The estimate on which this statement rests is based on the following ansatz for the wave function of the water molecule,

$$\psi_{\text{mol}}(X) = \frac{1}{N_{\text{mol}}} \frac{F_{5/2}(\eta_0, \kappa\rho)}{\rho^{5/2}} e^{-\kappa\rho} Y_{l\lambda}^{1M}(\hat{x}, \hat{y}). \quad (1)$$

Here we use, instead of the Jacobi variables $\{\vec{x}, \vec{y}\}$ of the $p + p + {}^{16}\text{O}$ system, the set of hyperspherical variables $X = \{\rho, \omega, \hat{x}, \hat{y}\}$ with $\rho = \sqrt{x^2 + y^2}$ being the hyperradius and $\omega = \arctan y/x$ the hyperangle. For the five angles in X , the notation $\Omega = \{\omega, \hat{x}, \hat{y}\}$ will be used, and the Coulombic potential of our problem is written in the form $V(X) = \mathcal{V}(\Omega)/\rho$. By F_ν the regular solutions of the hyperradial Schrödinger equation are denoted, and by $Y_{l\lambda}^{JM}(\hat{x}, \hat{y})$ the eigenfunctions of the total angular momentum operator. N_{mol} is a normalization factor, and $\kappa \sim \sqrt{|\varepsilon_{\text{mol}}|}$ represents the momentum corresponding to the binding energy ε_{mol} of the H_2O molecule; $\eta_0 = \mathcal{V}_0/2\kappa$ is a kind of Sommerfeld parameter, where \mathcal{V}_0 is obtained by averaging $\mathcal{V}(\Omega)$ with the angular part of $\psi_{\text{mol}}(X)$. The ansatz (1) takes correctly into account the Coulomb repulsion between the particles at small distances, as well as the geometric size of the water molecule.

For the description of the ${}^{18}\text{Ne}$ nuclear resonance state (1^-), we use the asymptotic form of the Coulombic three-body break-up function normalized to the nuclear volume,

$$\psi_{\text{res}}(X) = \frac{1}{N_{\text{res}}} \frac{f^1(\rho, \omega)}{\rho^{5/2}} Y_{l\lambda}^{1M}(\hat{x}, \hat{y}), \quad (2)$$

where

$$f^J(\rho, \omega) = \int d\hat{x} d\hat{y} \exp \left\{ iK\rho - i \frac{\mathcal{V}(\Omega)}{2K} \ln(2K\rho) \right\} Y_{l\lambda}^{JM}(\hat{x}, \hat{y}). \quad (3)$$

Here, $K \sim \sqrt{E}$ is the momentum corresponding to the energy E of the outgoing particles ${}^{16}\text{O} + p + p$.

Within the models (1) and (2) we find for the overlap integral the asymptotic estimate

$$I \sim \exp \left\{ -\frac{\pi}{2} \eta_K^0 \right\} \exp \left\{ i\eta_K^0 S \right\}, \quad (4)$$

where $\eta_K^0 = \mathcal{V}_{\text{min}}/2K$ is another kind of Sommerfeld parameter with \mathcal{V}_{min} being the minimal value of the angular part $\mathcal{V}(\Omega)$ of the total Coulomb potential. The phase S depends on \mathcal{V}_{min} and a parameter $\xi = K/\kappa$. From its definition follows that ξ can vary between $0 \leq \xi \leq \sqrt{\Gamma_p/|\varepsilon_{\text{mol}}|}$ with Γ_p being the width of the ${}^{18}\text{Ne}(1^-)$ level for the decay into the $p + p + {}^{16}\text{O}$ channel. When studying S as a function of ξ it turns out that there exists a wide subdomain of values of ξ in which $\text{Im } S < 0$ and $|\text{Im } S| > \frac{\pi}{2}$. That is, the overlap integral (4), and thus the transition rate

$$W = \kappa c |I|^2 \quad (5)$$

of the process $H_2O \longrightarrow {}^{18}\text{Ne}(1^-)$, increase exponentially with decreasing K (at small energies $E \sim K^2$). This is to be contrasted with the usual opposite behavior of transitions into short-ranged (non-resonant) nuclear states.

The above estimates imply that molecular water in the 1^- state has a non-vanishing probability to go over into the excited state ${}^{18}\text{Ne}(1^-)$, which then will decay either into the channel ${}^{17}\text{F} + p + Q_1$ ($Q_1 \cong 0.6$ MeV) or into the chain ${}^{18}\text{Ne}(1^-) \longrightarrow {}^{18}\text{Ne} + \gamma + Q_2 \longrightarrow {}^{18}\text{F} + e^+ + \nu$ ($Q_2 \cong 4.522$ MeV). Unfortunately, the partial widths of these two transitions are unknown and, therefore, it is impossible by now to estimate the whole energy release in the considered process of “burning” molecular water.

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